Propagation Behavior of Diverging Cylindrical Detonation in Mixture with Reactivity Change

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1 Introduction

In unconfined cylindrical and spherical geometries, the surface area of the detonation front continuously increases with radius as a diverging detonation. According to Lee [1], the number of cells must increase to keep the cell width constant as the detonation expands in a diverging detonation. Moreover, the generation of new transverse waves results in larger fluctuation of the shock front [1,2].

Previous studies [3] of a planar detonation wave in a constant area channel indicate that the generation of cells depends on the properties of the mixture, (e.g. effective activation energy). When the activation energy is large, generation and disappearance of cells occur more frequently so that irregular cellular structure is obtained. Irregular cellular detonations are less likely to be quenched with respect to expansion of a channel width than regular cellular detonations. In addition, previous research [4,5] on the initiation of diverging detonation indicate that activation energy affects the critical energy of direct initiated. However, the work on the effects of the activation energy on the propagation of diverging cylindrical (or spherical) detonation waves are still unclear.

The aim of this work is to clarify the propagation mechanism including local re-initiation and quenching of a cylindrical cellular detonation front. In this paper, the effect of the activation energy and shock front disturbances on propagation behavior of cylindrically expanding detonation waves is investigated.

2 Numerical Setup

The governing equation is two-dimensional compressible reactive Euler equation. The chemical kinetics is assumed to be governed by the one-step Arrhenius law. For the discretization of convection term and time integration, Yee's non-MUSCL type 2nd-order upwind TVD scheme and point implicit method treating only source term implicitly are used, respectively. Here, the dimensional variables in the governing equation are normalized by the ambient condition and half-reaction length, which is the distance required for mass fraction of reactant reducing from 1.0 to 0.5 in one-dimensional steady CJ detonation analysis and it is used as unit length. Grid resolution is set at 10 grid points per half-reaction length $L_{1/2}$. The

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computational domain with uniform and orthogonal grid system is set at maximum of $500L_{1/2}$. For the boundary condition, the mirror condition is used in the symmetric lines. In addition, chemical and fluid parameters are fixed as follows: specific heat ratio $\gamma = 1.2$ and heat release $Q = 22.5$. The activation energy E_a is chosen as a parameter in this paper, and $E_a = 10.0$, 17.0, 22.0 is used. According to neutral stability curves for one-dimensional planar CJ detonations by Eckett *et al*. [6], activation energies $E_a = 10.0$, 17.0, 22.0 corresponds to weakly unstable, relatively unstable, very unstable mixtures, respectively. Initial condition consists of two regions; the high-energy region with burned gas of initiation energy $E_s = 150\text{x}10^3$, $250\text{x}10^3$, $1100\text{x}10^3$ and the ambient region with uniformly premixed unburned gas.

3 Results and Discussions

The effect of the activation energy on the onset of diverging cylindrical detonation waves is investigated by using direct initiated detonation waves. Figure 1 shows shock pressure histories of x-axis line as parameters for $E_a = 10.0$, 17.0, and 22.0 in E_s = (a) $150\text{x}10^3$, (b) $250\text{x}10^3$, and (c) $1100\text{x}10^3$. As shown in Fig. 1, the activation energy affects the onset of directly initiated cylindrical detonations. The source energy for which the onset of a diverging cylindrical detonation requires tends to be higher as the activation energy increases. Figure 2 shows the mean cell width in the cases of (a) $E_s = 250$ and (b) $1100\text{x}10^3$. For $E_s = 250\text{x}10^3$, detonation initiation fails when $E_a = 22.0$ and cells could not be observed. Asahara *et al*. (2012) [7] described three propagation stages by the characteristic of cellular patterns. In the 1st stage, the average cell size increases as detonation front expands. In the transition stage, new transverse waves are generated drastically and make fine cellular pattern. In the 2nd stage, the detonation wave propagates with keeping the same average cell size by the generation of new transverse waves. As shown in Fig. 2, three propagation stages could be observed. Also, in $E_s = 1100\text{x}10^3$ and $E_a = 17.0$, and 22.0, the cell width in the 1st and transition stage is not so much different from each other. However, in the 2nd stage, the cell width becomes large as

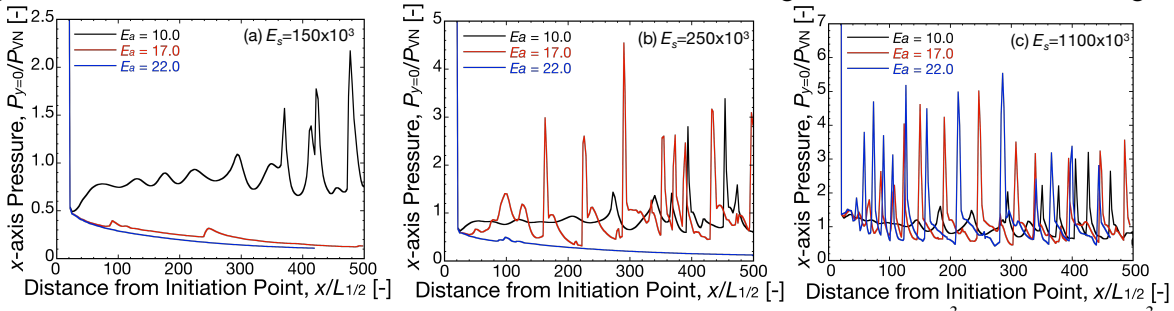

Figure 1. Shock wave pressure histories of x-axis line in the case of (a) E_s=150x10^3, (b) E_s=250x10^3, and (c) E_s=1100x10^3 (P_{VN}=20.03 denotes the value of von Neumann spike for CJ detonation)

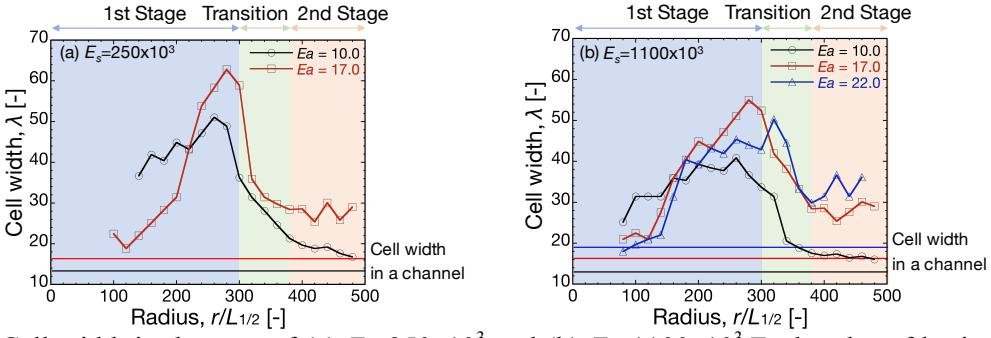

Figure 2. Cell width in the case of (a) E_s=250x10^3 and (b) E_s=1100x10^3.Each color of horizontal line is cell width of two-dimensional detonation propagating in a channel at same conditions

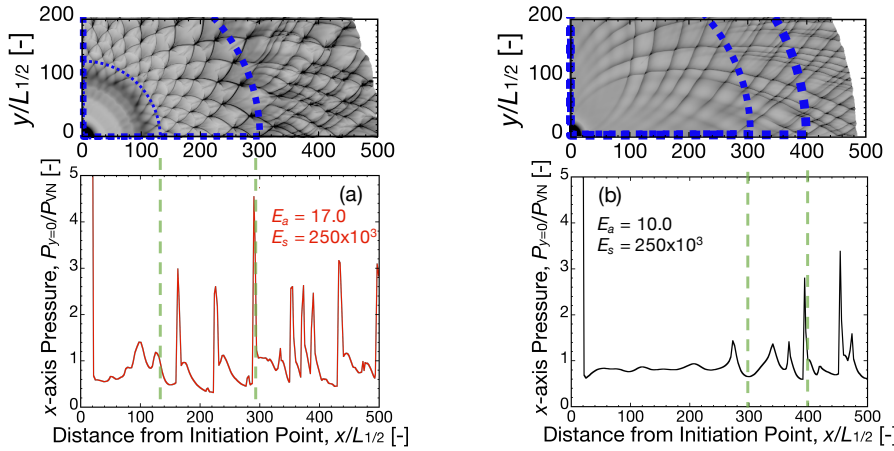

Figure 3. Maximum pressure history and shock pressure history of x-axis line in the cases of (a) $E_a = 17.0$ and $E_s = 250\text{x}10^3$ and (b) $E_a = 10.0$ and $E_s = 250\text{x}10^3$. Dotted blue and green line denote the position where activation energy changes in following results.

the activation energy increases. This trend corresponds to that of a planar detonation. Moreover, the cell width for $E_s = 250\text{x}10^3$ is the same as that for $E_s = 1100\text{x}10^3$ in the 2nd stage. Peak pressure values change at the transition stage in Figs. 1 and 2. In $E_a = 17.0$ and 22.0, peak pressure of the 1st stage is higher than that of the 2nd stage. On the other hand, in $E_a = 10.0$, peak pressure values of the 2nd stage is larger than that of the 1st stage, i.e. the instabilities of the shock front decrease at transition stage in $E_a = 17.0$ and 22.0 but increase in $E_a = 10.0$. From the above, activation energy affects both the onset and the propagation of cylindrical detonation waves and it is presumed that the source energy is more dominant for the propagation behavior in the 1st stage, and that activation energy has more effects on propagation behavior in the 2nd stage once detonation initiation is successful. Then, in order to investigate the effects of activation energy on cylindrical detonation propagation behavior, following method is introduced. Firstly, the detonation wave is initiated using $E_a = 17.0$ and 10.0 and $E_s = 250\text{x}10^3$ and $1100\text{x}10^3$. When detonation front reaches at blue or green dotted line shown in Fig. 3, activation energy is changed to 10.0, 17.0, and 22.0. In this report, $r/L_{1/2} = 125$, 300, and 400 are used as radii where the activation energy changes. $r/L_{1/2} = 125$ corresponds to changing E_a in the middle of the 1st stage, $r/L_{1/2} = 300$ corresponds to changing E_a in the early transition stage and $r/L_{1/2} = 400$ corresponds to changing E_a in the 2nd stage.

Figure 4 describes shock pressure histories of x-axis line and cell width in changing E_a from 17.0 to 10.0, 17.0, and 22.0 at $r/L_{1/2} = 125$. The initiation still fails in changing E_a to 22.0 and global propagation behavior in changing E_a in the 1st stage is almost the same as that in not changing E_a case. However, in the 2nd stage, Fig. 4(b) and (c) show that the cell width transition in $E_a = 10.0$, and 22.0 is closer to that in $E_a = 17.0$ than not changing E_a case. This indicates that propagation behavior of cylindrical detonation is not only affected by activation energy but also by small disturbances formed in the 1st stage.

Figure 5 shows shock pressure histories of x-axis line and cell width in changing E_a from 17.0 to 10.0, 17.0, and 22.0 at $r/L_{1/2} = 300$. Figure 6 also illustrates maximum pressure histories of $E_s = 250\text{x}10^3$. The characteristic of cell width in this case is the same as the former case. However, the blast wave propagates as detonation waves in $E_s = 250\text{x}10^3$ and $E_a = 22.0$ differing from the former cases (not changing E_a on the way and changing E_a in the 1st stage cases). Figure 7 illustrates the maximum pressure histories of changing E_a from 10.0 to each value. As shown in Fig. 7, the detonation fails to propagate in changing E_a from 10.0 to 22.0. This indicates that disturbances at the shock front affect more than the activation energy in the transition stage. Circumferential shock pressure at the radii where the activation energy changes are shown in Figs. 8 and 9. From Figs. 8 and 9, the number of transverse waves just before the transition stage is almost

the same independent of the activation energy. However, hereinafter pressure difference in the circumferential direction on the shock front and the nonuniformity due to the shock front shape formed in the 1st stage are considered as shock front instabilities, this instability is larger in E_a = 17.0 than in the case of E_a = 10.0. New transverse waves must generate rapidly and bifurcate into fine cells in the transition stage to propagate as detonations. According to Asahara *et al*. [7], the mechanism of cell bifurcation in the transition stage is that small disturbances in the vicinity of a shock front due to expansion interferes with sub-transverse waves and grow into new transverse waves. As shown in Fig. 10, even if the conditions are the same as to E_s = 250x10^3 and changing E_a from 10.0 to 22.0, whether the detonation wave continues to propagate or is quenched depends on the radius where E_a changes from 10.0 to 22.0.

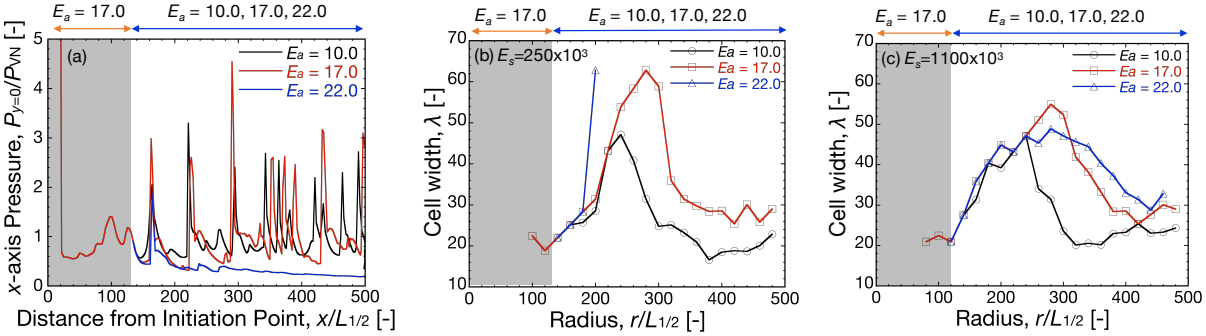

Figure 4. Cases of changing the activation energy from E_a = 17.0 to each value at radius $r/L_{1/2}$ = 125, (a) Shock wave pressure history of x-axis line of E_s = 250x10^3, and Cell width of (b) E_s = 250x10^3, and (c) E_s = 1100x10^4

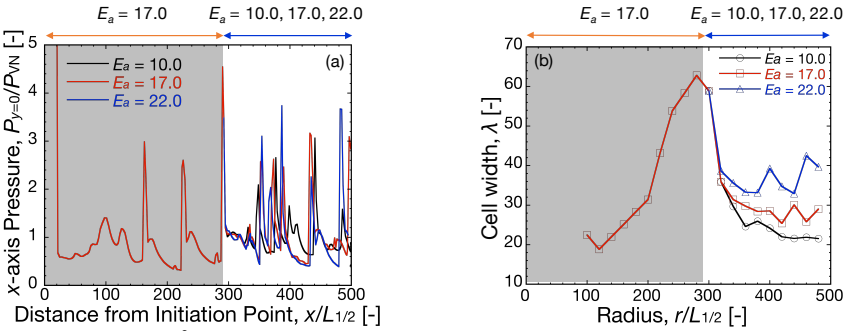

Figure 5. Cases of E_s = 250x10^3 and changing the activation energy from E_a = 17.0 to each value at radius $r/L_{1/2}$ = 300, (a) Shock wave pressure history of x-axis line and (b) Cell width

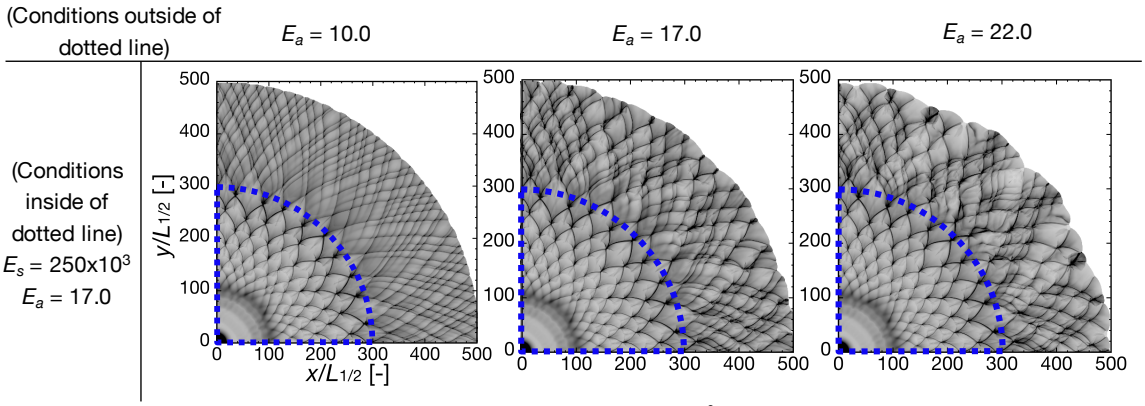

Figure 6. Maximum pressure history in the cases of E_s = 250x10^3 and changing the activation energy from E_a = 17.0 to each value at radius $r/L_{1/2}$ = 300

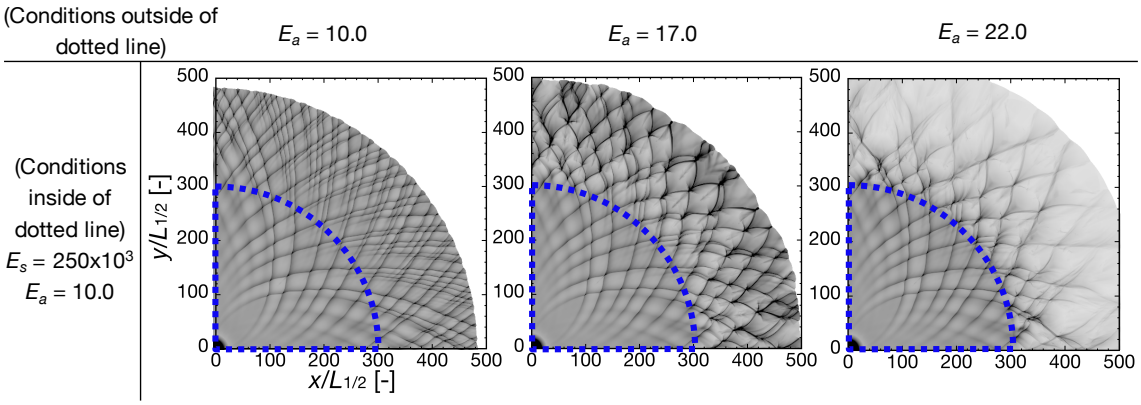

Figure 7. Maximum pressure history in the cases of $E_s = 250\text{x}10^3$ and changing the activation energy from $E_a = 10.0$ to each value at radius $r/L_{1/2} = 300$

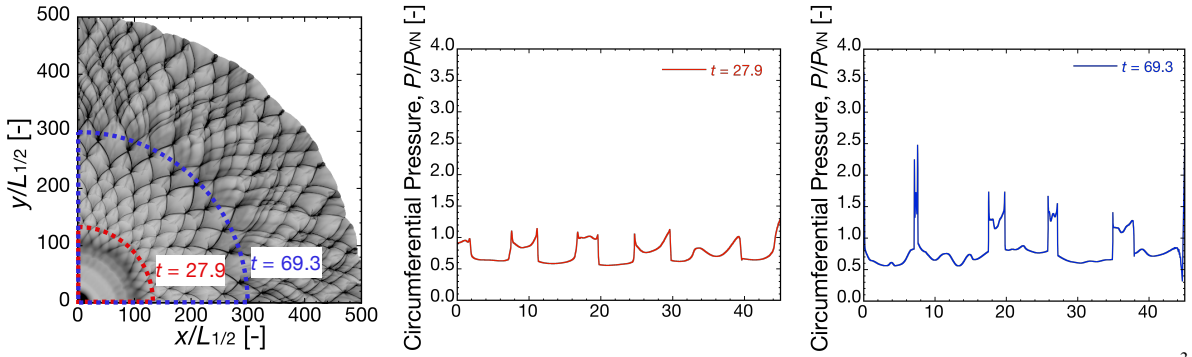

Figure 8. Shock circumferential pressure versus angle at $t = 27.9$, 69.3 in $E_a = 17.0$ and $E_s = 250\text{x}10^3$

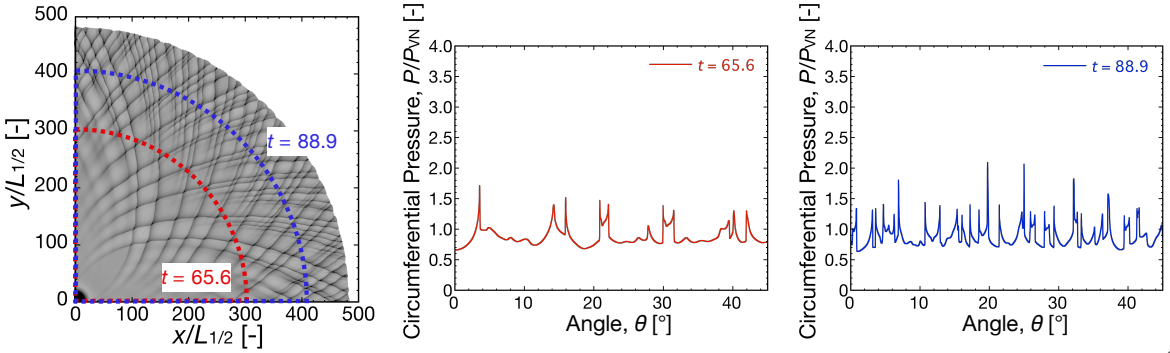

Figure 9. Shock circumferential pressure versus angle at $t = 65.6$, 88.9 in $E_a = 10.0$ and $E_s = 250\text{x}10^3$

Considering the above, the generation of new transverse waves in the transition stage is more affected by the shock front instabilities formed in the 1st stage than by the activation energy. The detonation front once propagates into the 2nd stage, it is considered that the activation energy is more dominant for cylindrical detonation propagation behavior than both the source energy and the shock front instabilities. For a planar detonation case, irregular cellular detonations, i.e. in the lower activation energy, are less likely to be quenched with respect to expansion of a channel width than regular cellular detonations. However, for diverging cylindrical detonations in the 1st and transition stage, it is easier for diverging cylindrical detonations to propagate in the lower activation energy.

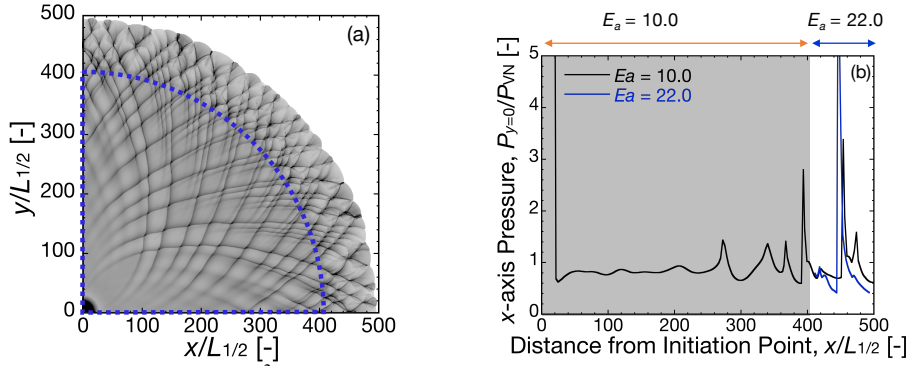

Figure 10. In the case of $E_s = 250\text{x}10^3$ and changing E_a from 10.0 to 22.0 at radius $r/L_{1/2} = 400$, (a) maximum pressure history and (b) shock pressure history of x-axis line

4 Conclusion

Two-dimensional numerical simulations with one-step chemical reaction are carried out to clarify the effect of activation energy on a diverging cylindrical detonation propagation. Firstly, the directly initiation study shows that the activation energy affects both the onset and propagation behavior of the detonation. The critical source energy for weakly unstable mixtures tends to be lower than that value of unstable mixtures. Although the activation energy has an effect on both the onset and propagation behavior of diverging detonations, propagation behavior in the 1st stage depends more on the source energy. Secondly, in the transition stage, it is considered that shock front instabilities formed in the 1st stage affect the propagation behavior more than the activation energy and the source energy. In the 1st and transition stage, it is easier for diverging cylindrical detonations to propagate in the lower activation energy. Finally, once the detonation propagates into the 2nd stage, the activation energy is more dominant for the diverging cylindrical detonation propagation behavior.

References

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